UNDERSTANDING THE TUNNELING PATTERNS OBSERVED IN THE BROADBAND ROTATIONAL SPECTRA OF DIPHENYL ETHER AND ITS COMPLEX WITH ONE WATER MOLECULE

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Diphenyl ether ($C_{12}H_{10}O$) is a flexible molecule, and it offers two types of competing binding sites to form non-covalently bound complexes, the ether oxygen and the aromatic π system. Its dimer and complexes with water, methanol, *tert*-butyl alcohol and adamantanol have been investigated with broadband rotational spectroscopy [1,2]. Using this method, we were able to accurately reveal the structures and internal dynamics of these weakly bound molecular clusters isolated in the gas phase. The spectrum of the DPE monomer shows tunneling splitting of each transition due to the concerted internal rotation of both of its phenyl rings around C-O bonds. In the weakly bonded complexes, the tunneling splitting of DPE is quenched due to intermolecular interaction. However, in one of the hydrogen-bond complexes of DPE with one water molecule, the *a*-type transitions are split. This is due to a concerted motion comprised of the tunneling of the DPE monomer and the internal motion of the water molecule. The analysis of the motions involved in the splitting pattern in DPE and its one water complex will be presented and discussed.

[1]M. Fatima et al., Angew. Chem. Int. Edit., 58 (2019), 3108.

[2]F. Dietrich et al., Angew. Chem. Int. Edit., 57 (2018), 9534.